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Particle model for fluid membrane with fluctuating spontaneous curvature

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粒子を用いた膜の簡単な数学的模型を提案する。粒子は膜の一部を表現していると考え、ディレクタ S と自発曲率の極性を表す p を属性として持っているとする。自発曲率の揺らぎを取り入れると、膜が柔らかくなり、さらに揺らぎが大きい場合には自発的にミセルが生まれる。また、異方性相互作用の大きさを弱めると、多重膜のベシクルが転移を通して現れる。

Extending the pioneering particle model by Drouffe et al.[1], we present a simple mathematical membrane model which consists of particles with polarities p of spontaneous curvature and directors $\mathbf{S}$ ($|\mathbf{S}| = 1$) of the membrane. A particle in the model is considered to represent one small part of the membranes. The shape of the particle labeled by i is assumed to be a sphere, but the interaction between neighboring particles is anisotropic through the directors $\mathbf{S}_i$, the polarity p_i and the position difference $\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$ between two particles i and j. The interaction potential of the model is written by

$$\begin{aligned} F &= \frac{1}{2}\sum_{i,j}\{V_0(r_{ij}) - V_1(r_{ij})(1 + hp_ip_j\mathbf{S}_i \cdot \mathbf{S}_j)\} \\ &\quad + D\sum_{i,j} V_1(r_{ij})\left\{(\mathbf{S}_i \cdot \tilde{\mathbf{r}}_{ij})^2 + p_i\mathbf{S}_i \cdot \tilde{\mathbf{r}}_{ij}\right\} + \frac{K}{2}\sum_i \frac{p_i^2}{1-(p_i/X)^2}, \end{aligned} \tag{1}$$

where $r_{ij} = |\mathbf{r}_{ij}|$ and $\tilde{\mathbf{r}}_{ij} = \mathbf{r}_{ij}/r_{ij}$. The first term of Eq.(1) indicates the isotropic interaction where two particles are attracted by the negative long range potential $-V_1(r)$ and are repelled by the repulsive short-range potential $V_0(r)$. The attractive ferromagnetic interaction between neighboring spins $p_i\mathbf{S}_\mathrm{i}$ and $p_j\mathbf{S}_\mathrm{j}$ is included if h is not zero. The second term of Eq.(1) implies the anisotropic interaction whose strength can be adjusted by the parameter D. If the polarity p_i is not zero, $p_i\mathbf{S}_i \cdot \tilde{\mathbf{r}}_{ij}$ plays the role of spontaneous curvature. The last term of Eq.(1) is added to suppress the growth of the polarities p_i smaller than the saturation value X.

Simulations are performed by using the Langeven dynamics, and the bending modulus for the membrane was obtained by analyzing the fluctuation spectrum of the lamella without lateral tension. The results are shown in Fig.1 for various K and h, and the relation between them are written by

$$\kappa = \kappa_0\Big(1 - \frac{c_0}{K - c_1h}\Big), \tag{2}$$

which are confirmed by simulations and analytic calculations. Decreasing K, the amplitude of fluctuation of the polarity p increases, and the bending modulus decreases. With small K or

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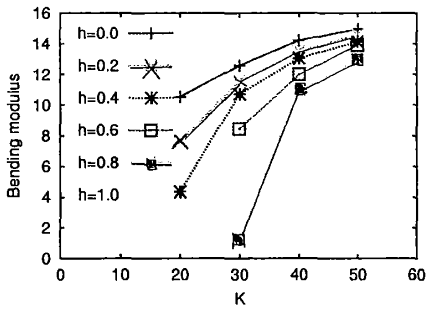

Figure 1: Bending modulus

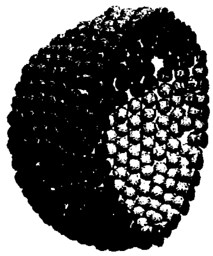

Figure 2: Fluid vesicle

large h satisfying $\kappa < 0$ estimated by Eq.(2), vesicles or micelles appear spontaneously from a uniform distribution of particles at initial time.

Starting from the initial positions of particles on an icosahedron, fluctuating vesicles are obtained. Fig.2 shows a snapshot of the fluctuating vesicles whose membranes is in fluid state. Increasing the temperature, the state of the membrane changes from crystal to fluid at a certain temperature. In the interaction energy described by Eq.(1), the parameter D indicates the

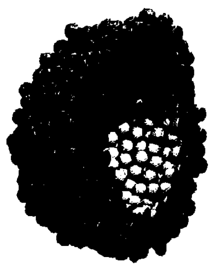

Figure 3: Multi-layered vesicle

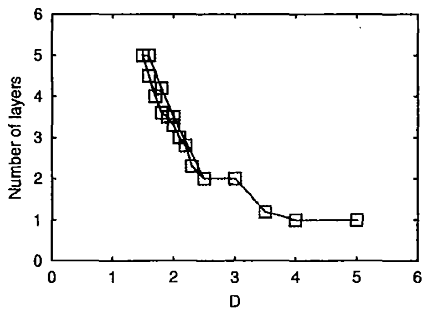

Figure 4: Number of layers.

strength of the anisotropic interaction between particles with directors **S**. If D is small enough, the interaction between particles is almost isotropic, and a normal phase diagram with solid droplets, liquid droplets and gas will be obtained depending on the temperature. Increasing D, layered structures begin to appear in the system. We observed a reversible phase transition between multi-layered membranes in the process that D is decreased from a value at which a monolayer vesicle is stable, and then D is increased until a monolayer vesicle reappears. Fig.3 shows a snapshot of a multi-layered vesicle, where three or four layers are observed in the shell, and there is a hole at the center of the vesicle. The phase diagram of the multi-layered membranes is shown in Fig.4

1) J.-M. Drouffe, A. and C. Gaggs, S. Leibler, Science **254**,1353 (1991).

2) T. Kohyama, in preparation.